Graph networks for molecular design

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Abstract

Deep learning methods applied to chemistry can be used to accelerate the discovery of new molecules. This work introduces GraphINVENT, a platform developed for graph-based molecular design using graph neural networks (GNNs). GraphINVENT uses a tiered deep neural network architecture to probabilistically generate new molecules a single bond at a time. All models implemented in GraphINVENT can quickly learn to build molecules resembling the training set molecules without any explicit programming of chemical rules. The models have been benchmarked using the MOSES distribution-based metrics, showing how GraphINVENT models compare well with state-of-the-art generative models. This work compares six different GNN-based generative models in GraphINVENT, and shows that ultimately the gated-graph neural network performs best against the metrics considered here.